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Simulation of water purification using magnetically ultra-responsive micro- and nanoscavengers

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ABSTRACT

Access to clean water is one of the challenges of the 21st century. Thus water purification is inevitable. One method of water treatment is purification by magnetic particles in the presence of magnetic field. The contaminants are attached to the magnetic particles and then by applying a magnetic field, magnetic particles and, thus, the pollutants can be collected. For the optimal design of a water treatment system, the effect of important parameters in the design, such as magnetic fields, particle size, and Reynolds number are determined numerically by modeling and simulating the water treatment process. Two methods are used to create the magnetic field: permanent magnet and coils. It is shown that there is very little difference in the collection efficiency. Particle size is varied from micrometers to nanometers. In general, the collection efficiency increases by increasing the particle diameter and decreasing the Reynolds number. For example, it is shown that with a magnetic field of strength 0.05 T and Reynolds number of 100, particles with a diameter of 30 micrometers and above are collected completely. However, with decreasing particle diameter to the nanometer, collection efficiency finds a sharp drop. Using baffles to shift the particles toward regions with stronger fields, it is possible to increase the collection efficiency for nanoparticles.

1. Introduction

Water is the most important aspect of the human life and development of civilization. Access to clean and usable water resources is one of the most important goals of human beings and clean water accessibility is considered as the most important challenge in the 21 st century. The main sources of drinking water are including groundwater, lakes, seas, and rain. Nowadays, the severe crisis in relation to water resources is ahead of us. According to the World Health Organization (WHO), about 780 million people do not have access to reliable sources of drinking water all over the world [1]. Today, unfortunately, different industries, bring many pollutions such as industrial waste, toxic substances, heavy metals, alkalis, toxic gasses, radioactive materials, pathogenic microorganisms, fats, and oils into freshwater resources; thus, unclean water purification is inevitable [2].

In general water purification methods are classified into six groups: Adsorption, biotechnology, catalytic processes, membrane processes, radiation processes and processes using the magnetic field. Magnetism is the only physical property that independently affects the physical properties of contaminants and, thus, helps water purification. Water treatment using magnetic field has been developed over decades. For example, Mahmoud et al. [3] used magnetic treatment for hard water. They found that the anti-scaling efficiency of the applied permanent magnets was about 45%. High gradient magnetic separation (HGMS), is a method which commonly used in magnetic separation. HGMS can separate paramagnetic materials with sizes less than one micrometer at a rate equal to several hundred faster than the old methods [4]. Yano et al. used HGMS for the separation of steel waste. They found that the use of HGMS in terms of operational costs and space requirements is better than the sand filter [5]. Svoboda [6] presented a model for describing particles behavior in high gradient magnetic separation. Moeser et al. [7] have studied high gradient magnetic separation of magnetic nanoparticles with the size of about 8 nm. Collection of magnetic nanoclusters with HGMS has been studied experimentally by Ditsch et al. [8]. They have developed the method so that nearly all clusters with sizes of more than 50 nm have been collected ($>$ 99.9%). Shape and strength of the magnetic field source are the main parameters which affect separation. Li et al. [9] have studied the effect of different shapes of magnetic sources in HGMS theoretically.

In addition to HGMS methods, some simple ways are proposed using the single magnet. For example, Gabrielli et al. [10] have built a household magnetic device for water treatment using the permanent magnet. Eskandarpour et al. [11] have studied performance, recovery, and design of superconducting magnetic filter for wastewater

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treatment. Magnetic separation is a known method for ion metal removal. Many works have been done in this field [12]. Broomberg et al. [13] have reviewed works which have been done for removing metal ion using magnetic separation. Mehta et al. reviewed the works done in the field of magnetic adsorbents [14].

On the other hand, using micro- and nanoparticles is a developing method for water purification and many works have been conducted [1,15]. One type of particle which is used in water purification is magnetic particle [2,16–20]. Shen et al. [21] used Fe3O4 nanoparticles for polluted water purification. They showed that this particle is suitable for removing of metal ions like Ni, Cu, Cd, and Cr. Also, they found that the adsorption capacity of Fe3O4 particles increased when the particle size decreased or the surface area increased.

Many efforts have been made to improve particles properties and, thus, improve the treatment efficiency [22]. One of them is coating particles with silver. Silver coated magnetic particles have received much attention due to their antimicrobial effects [23–30]. Zhang et al. [31] used multilayer magnetic particles with the Ag-coated shell to remove pathogen and heavy metals from water. They used a permanent magnet to collect the magnetic particles. The collection efficiency was very good and within 5 min over 99 percent of particles were collected. The contaminants stick to particles and hence using a permanent magnet can collect particles and contaminants as well.

With all the above explanations using magnetic particles to adsorb contaminants such as metal ions and pathogen, is a robust way for water purification. The good contaminant absorption of magnetic particles, their very rapid response to magnetic field in order to collect them and capability of being recovered in any purification cycle are the reasons which stimulate researchers and water purification industries to use magnetic particles in water treatment. But challenges in post-treatment remain. It is very important to know how magnetic field strength, fluid flow, and particle diameter affect collection efficiency of the magnetic particle. However, to the best of our knowledge, no reliable experimental or numerical work on the collection of these magnetic particles has been reported yet.

Many factors should be count on to achieve an optimum water purification system such as particles size, magnetic field strength. In the present work, we attempt to determine these factors to design the required purification system. We employ a finite element model to simulate the collection process and understand the effects of each parameter. The magnetic field and the laminar flow are solved in the first step. Forces acting on each particle are calculated at every time step. The motion of particles is a time-dependent process. Thus, the unsteady particle motion is studied in the next step. The values obtained from the first step are used as the input values for the second step. Then, the position of each particle is obtained and the process is repeated until the end of the simulation. The results show that the collection efficiency increases by increasing the particle diameter and decreasing the Reynolds number. The details of the modeling, solution, results, and discussions will be presented in the next sections.

2. The system geometry

In water treatment by micro- and nanomagnetic particles, the particles enter the tank in which infected water is available. The particles are given a little time to collect pollutants and contaminants, and then they depart from the tank. In the outlet pipe magnetic particles, which contain contaminants including bacteria and germs, are separated from the water using a magnetic field; in this way the purified water is obtained. A schematic representation of the system is shown in Fig. 1.

Magnetic particles are coated with silver to collect more pollutants like bacteria and pathogen besides heavy metals (Fig. 2a). Then, by applying the magnetic field, magnetic particles and, thus, the attached contaminants are collected; hence, the water is purified from pollution. Forces exerted on the particles and the path of the particles during collection are shown in Fig. 2b and c.

In the present study, the Reynolds number is considered 100, thus, the flow regime is laminar. The purpose of the simulations is to investigate the main parameters which affect particles collection for designing an optimum system to maximize attraction of the magnetic particles used in the water treatment.

3. Governing equations

Velocity field of the fluid flow is obtained from the continuity and the Navier-Stokes equations:

$$\nabla.\, \vec{V} = 0 \tag{1}$$

$$\frac{D\vec{V}}{Dt} = \upsilon \nabla^2 \vec{V} + \vec{g} \tag{2}$$

where V and υ are the flow velocity and kinematic viscosity, respectively.

The magnetic field is described using Maxwell's equations:

$$\vec{J} = \nabla \times \vec{H} \tag{3}$$

$$\nabla \times \vec{B} = 0 \tag{4}$$

$$\vec{B} = \mu_0(\vec{H} + \vec{M}) = \mu_0(\vec{H} + \chi\vec{H}) \tag{5}$$

where J, H, and B are the current density, magnetic density, and magnetic field, respectively. Also, μ_0, M and χ represent the vacuum permeability, material magnetization and magnetic susceptibility, respectively.

Newton's second law describes the momentum of a particle as below:

$$\vec{F} = \frac{d\,\vec{u_p}}{dt} \tag{6}$$

$$\vec{F} = \vec{F_D} + \vec{F_M} + \vec{F_B} \tag{7}$$

where $\vec{F}$ is the net force acting on the particle (Fig. 2).

$\vec{F_D}$ is the drag force which is obtained by following equations:

$$F_D = \frac{1}{\tau_p} m_p(u - v) \tag{8}$$

$$\tau_p = \frac{\rho_p d_p^2}{18\mu} \tag{9}$$

where μ is the dynamic viscosity of water, d_p and ρ_p are particle's diameter and density, respectively. $u - v$ represents the particle's relative velocity and F_M is the magnetic force acting on the particle, which is calculated by the following relation:

$$F_M = 2\pi r_p^3 \mu_0 \mu_{r,f} K \nabla H^2 \tag{10}$$

where H is magnetic field intensity, μ_0 and $\mu_{r,f}$ are the vacuum and relative permittivity, respectively.

F_B is the Brownian force and is obtained from the following equation:

$$F_B = \zeta \sqrt{\frac{12\pi k_B \mu T r_p}{\Delta t}} \tag{11}$$

where T is absolute temperature, k_B is the Boltzmann constant, Δt is time step and ζ is the Gaussian random number with zero mean and unit standard deviation.

Thus, Eq. (6) can be rewritten as:

$$m_p \frac{d\,\vec{u_p}}{dt} = \frac{1}{\tau_p} m_p(u - v) + 2\pi r_p^3 \mu_0 \mu_{r,f} K \nabla H^2 + \zeta \sqrt{\frac{12\pi k_B \mu T r_p}{\Delta t}} \tag{12}$$

The collection efficiency is defined as below: